A Supplementary Document of "A Systematic Approach for the Construction of Definitive Screening Designs"

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S1 Proof of Theorem 1

Consider that C has the following structure:

$$\mathrm{C} = \begin{pmatrix} 0 & \delta & \vec{\delta'} & \vec{\delta'} \\ 1 & 0 & \vec{\delta'} & -\vec{\delta'} \\ \vec{1} & \vec{1} & T & S\delta \\ \vec{1} & -\vec{1} & S & -T\delta \end{pmatrix} \tag{S1.1}$$

Since S is circulant by Lemma 1 and T is also circulant by Lemma 2 under condition (1), we have

$$\mathrm{C}'C = \begin{pmatrix} 2n+1 & 0 & \vec{1'}(\delta+s+t) & \vec{1'}(-\delta+s\delta-t\delta) \\ 0 & 2n+1 & \vec{1'}(\delta-s+t) & \vec{1'}(1+s\delta+t\delta) \\ \vec{1}(\delta+s+t) & \vec{1}(\delta-s+t) & 21_{n\times n}+(T^2+S^2) & 0 \\ \vec{1'}(-\delta+s\delta-t\delta) & \vec{1}(1+s\delta+t\delta) & 0 & 21_{n\times n}+(T^2+S^2) \end{pmatrix} \tag{S1.2}$$

where $\vec{1}$, δ, s and t are defined in section 3, $1_{n\times n}$ is a $n\times n$ matrix that all entries are 1. Since S and T are circulant, ST is circulant and $ST = TS$. This leads to the zeros in the $(3;4)$- and $(4;3)$-locations of $C'C$, which are $(TS\delta - ST\delta)$ and $(ST\delta - TS\delta)$ before evaluations. If C is a conference matrix, it must fulfill $C'C = (m-1)I$, where $m-1 = 2n+1$ in our case. Therefore, C'C has to be diagonal, i.e., all off-diagonal locations have to be all zeros. For those locations with s and t, when n is even ($\delta = 1$), equations in those locations are reduced to a problem of solving the simultaneous equations $1+s+t=0$ and $1-s+t=0$, and the solution falls on the linear line $s+t=-1$. The preferred choice of $s=0$ and $t=-1$ guarantees the balanced selection of $+1$ and -1 in S. When n is odd ($\delta = -1$), the solution to the simultaneous equations $-1+s+t=0$ and $1-s+t=0$ falls on the linear line $s+t=1$. The preferred choice of $s=1$ and $t=0$ guarantees the balanced selection of $+1$ and -1 in T. These preferred choices of solutions are condition (2). Lastly, both $(3;3)$- and $(4;4)$-locations have to be diagonal matrices with diagonal entries $2n+1$, denoted as $I_n(2n+1)$. In order to achieve this goal, $T^2+S^2 = I_n(2n+1) - 21_{n\times n}$. The resulting matrix has $2n-1$ in its diagonal entries and -2 in its off-diagonal entries. The values in the diagonal entries are obvious and they are $\sum_{i=1}^{n}(t_i^2+s_i^2)$. The first term sums up to be $n-1$ because $t_1 = 0$ and the second term sums up to be n. The values in the off-diagonal entries of T^2+S^2 are not trivial. First, notice that T and S are symmetric and circulant, so do T^2, S^2 and T^2+S^2. This reduces the problem to that for $k = 1;\ldots;n-1, all(1;1+k)-$ entries are -2. Applying condition (3) with $k=1$ to $(1;2)$-entry leads to

$$(t_1t_2+s_1s_2)+(t_2t_3+s_2s_3)+\cdots+(t_nt_1+s_ns_1) = -2. \tag{S1.3}$$

Applying condition (3) with $k=2$ to $(1;3)$-entry leads to

$$(t_1t_3+s_1s_3)+(t_2t_4+s_2s_4)+\cdots+(t_nt_2+s_ns_2) = -2. \tag{S1.4}$$

By repeatedly applying condition (3) to all $(1;1+k)$-entry lead to -2 for all integers $k < \frac{n+1}{2}$. Furthermore, since all values in $(1;1+k)$-entries are equal to those in $(1;n+1-k)$-entries, this means the first column of T^2+S^2 is a vector $(2n+1;-2;\ldots;-2)$. The circulant property of T^2+S^2 ensures that all off-diagonal entries are -2. This completes the proof of Theorem 1, showing that C is a $(2n+2)\times(2n+2)$ conference matrix.

S2 Proof of Theorem 3

Consider that C has the following structure:

$$C = \begin{pmatrix} 0 & -\vec{\delta} & -\vec{\delta} \\ \vec{1} & T & S\delta \\ -\vec{1} & S & -T\delta \end{pmatrix} \tag{S2.1}$$

Since S is circulant by Lemma 1 and T is circulant by Lemma 2 under condition (1), we have

$$\mathrm{C}'C = \begin{pmatrix} 2n & \vec{1}'(-s+t) & \vec{1}'\delta(s+t) \\ \vec{1}(-s+t) & 1_{n\times n} + (T^2+S^2) & 1_{n\times n} \\ \vec{1}\delta(s+t) & 1_{n\times n} & 1_{n\times n} + (T^2+S^2) \end{pmatrix} \tag{S2.2}$$

where $\vec{1}$, δ, s and t are defined in section 3, $1_{n\times n}$ is a $n\times n$ matrix that all entries are 1. Similar to the argument int he proof of Theorem 1, the circulant properties of

S and T implies $TS = ST$, and this leads to $1_{n\times n}$ in the $(2;3)$- and $(3;2)$-locations of $C'C$, where the cancellations of (STδ -TSδ) and $(TS\delta - ST\delta)$ take places respectively. Under condition (2), no matter n is even or odd, $-s+t = \delta(s+t) = -1$. This means all entries in the first row and the first column, except the $(1;1)$-location, are -1. Lastly, to evaluate $1_{n\times n} + (T^2 + S^2)$ in the $(2;2)$- and $(3;3)$-locations, we borrow some results in the proof of Theorem 1. When condition (3) holds, $T^2 + S^2$ is a $n \times n$ matrix such that its diagonal entries are $2n-1$ and its off-diagonal entries are -2. When a $1_{n\times n}$ is added, the resulting matrix has its diagonal entries $2n$ and its off-diagonal entries -1, which is the$A$ matrix defined in Theorem 3. The proof is completed.

S3 Proof of Theorem 4

The goal is to derive the determinant of $C'C$ and show that they can be expressed in the form of the total product of two sequences. The simplest way to calculate the determinant of a square matrix is to rewrite the matrix into reduced row echelon form, which is a upper triangular matrix. Then the determinant is simply the trace of the matrix.
About the three sequences, the elements of $\{a\}$ are the first $n+1$ diagonal entries of the resulting upper triangular matrix, the elements of $\{o\}$ are the second to the $(n+2)$th entries of the last column of the matrix and the last $n-1$ elements of fbg are the last $n-1$ diagonal entries of the resulting upper triangular matrix. Notice that the first diagonal entry is $2n$. To derive the initial condition, let R_1 and R_2 be the first and second row of $C'C$. By substituting $(-1)R_1/(2n) - R_2$ to R_2, the first entry becomes zero and the second entry, which is a_1, becomes $2n - 1/(2n)$. The last entry in R_2, which is o_1, becomes $1 - 1/(2n)$. b_1 is implicit at this point, is set to be equivalent to a_1. Following the standard operations to reduced row echelon form, two observations are important. First, at the i stage, i.e., R_{i+1} row is always substituted by $(k_i^2)R_i/a_i$ for $i \le n+1$, or $(k_i^2 R_i)/b_{i-1}$ for $i > n+1$, where k_i is the entry below and right to the diagonal entry of R_i. Furthermore, for $i \le n+1$, $a_{i-1} - k_i = 2n+1$, and for $i > n+1$, $b_{i-1} - k_i = 2n+1$. These two facts help in simplifying the derivations. Consider the standard operation to reduced row echelon form is done at i stage, a_i can be expressed as $a_{i-1} - \frac{k_i^2}{a_{i-1}}$. The substitution $k_i = a_{i-1} - (2n+1)$ and some algebra lead to $a_i = (2n+1)(2 - \frac{2n+1}{a_{i-1}})$. Next, o_i can be expressed as $o_{i-1} - \frac{k_i o_{i-1}}{a_{i-1}}$. The substitution of k_i and some algebra lead to $o_i = o_{i-1}(\frac{2n+1}{a_{i-1}})$.

The derivation of the first $n+1$ elements in $\{b\}$ is not as trivial as the other two because it is not explicitly shown in the final result. Notice that these $n+1$ elements track the change of last $n-1$ diagonal entries during the first $n+1$ operations. With this concept, any of the last $n-1$ rows, instead of the R_{i-1}, is considered in the i stage. Then b_i can be expressed as $b_{i-1} - \frac{o_i^2}{a_{i-1}}$. The substitution of $o_{i-1} = \frac{o_i a_{i-1}}{2n+1}$ and some algebra lead to $b_i = b_{i-1} - \frac{o_i^2 a_{i-1}}{(2n+1)^2}$ for $i \le n+1$. For the rest $n-1$ elements of $\{b\}$, similar idea from the elements of $\{a\}$ applies and thus $(2n+1)(2 - \frac{2n+1}{b_{i-1}})$.

At this point, the matrix $C'C$ becomes reduced row echelon form and it is a upper triangular matrix, and its diagonal elements are $(2n, a_1, \ldots, a_{n+1}, b_{n+2}, \ldots, b_2 n)$. Then the determinant of $C'C$ is simply the product of all thse diagonal elements, and thus the D-effiency of D can be obtained. This completes the proof.